CRYSTAL STRUCTURES

Second Edition

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VOLUME 4

Miscellaneous Inorganic Compounds, Silicates, and Basic Structural Information

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Preface

The presentation of data in this volume follows without significant change the pattern established in preceding volumes of this edition. As in Volume V, which was issued earlier, right-hand axes are used in all new drawings.

Since this edition was planned, it has been decided not to enlarge its scope by including intermetallic compounds. Instead, Chapter XIII is devoted to a very abbreviated statement of basic ideas about symmetry and valence. The writer has found that there are many people wishing to use structural data whose training has not prepared them to read with understanding the descriptions of structure now standard. Chapter XIII aims to give this information in as condensed a form as possible. Considering the rapidity with which valence theory is developing, its discussion of valence will undoubtedly seem inadequate to chemists concerned with the subject. In the writer's experience, however, there is little middle ground between a cursory statement such as that given here and a treatment, dealing mostly with organic structures, too long and detailed to be appropriate to the present series.

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TABLE XI,45

Positions and Parameters of the Atoms in $PbBi_2Nb_2O_9$

Atom	Position	x	y	z
Pb	(4a)	0	0	0.500
Bi	(8c)	0	0.50	0.200
Nb	(8c)	0	0.50	0.422
O(1)	(4a)	0	0	0.00
O(2)	(8b)	$^1/_4$	$^1/_4$	0.25
O(3)	(8b)	$^1/_4$	$^1/_4$	0.079
O(4)	(8b)	$^1/_4$	$^1/_4$	−0.079
O(5)	(8c)	0	0.50	0.156

with the parameters of Table XI,45.

This structure, like those of $Bi_4Ti_3O_{12}$ (**IX,f12**) and $BaBi_4Ti_4O_{15}$ (**XI,13**) is built up of alternating Bi_2O_2 and perewskite-like layers.

The following compounds are isostructural:

Crystal	a_0, A.	b_0, A.	c_0, A.
$BaBi_2Nb_2O_9$	5.533	5.533	25.55
Bi_3TaTiO_9	5.402	5.436	25.15
Bi_3TiNbO_9	5.409	5.453	25.16
$CaBi_2Nb_2O_9$	5.435	5.485	24.87
$CaBi_2Ta_2O_9$	5.435	5.468	24.97
$SrBi_2Nb_2O_9$	5.504	5.504	25.05
$SrBi_2Ta_2O_9$	5.509	5.509	25.06
$KBi_4(Nb_2O_9)_2$*	5.506	5.506	25.26
$NaBi_4(Nb_2O_9)_2$*	5.47	5.47	26.94

*Two molecules per cell.

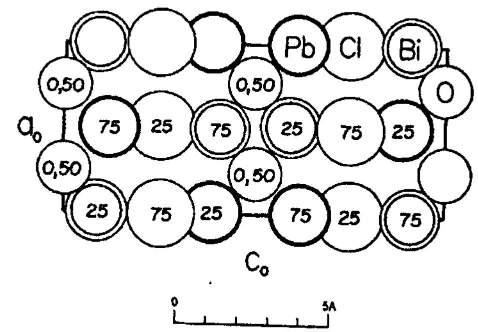
At elevated temperatures a_0 approaches b_0 and the symmetry of these compounds becomes tetragonal.

XI,78. The oxychloride mineral *perite*, $PbBiO_2Cl$, is orthorhombic with a tetramolecular unit of the edge lengths:

$$a_0 = 5.627(50) \text{ A.}; \quad b_0 = 5.575(20) \text{ A.}; \quad c_0 = 12.425(90) \text{ A.}$$

Its space group is V_h^{17} (*Bmmb*) with atoms in the positions:

Pb: (4c) $\pm(0\,^1/_4\,u;\ ^1/_2,^1/_4,u+^1/_2)$ with $u = 0.385$
Bi: (4c) with $u = 0.090$
Cl: (4c) with $u = 0.75$
O: (8e) $\pm(u00;\ u\,^1/_2\,0;\ u+^1/_2,0,^1/_2;\ u+^1/_2,^1/_2,^1/_2)$



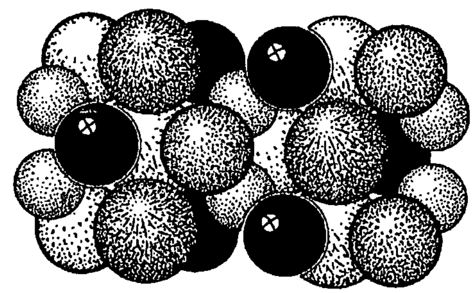


Fig. XI,60a (top). The orthorhombic structure of $PbBiO_2Cl$ projected along its b_0 axis.

Fig. XI,60b (bottom). A packing drawing of the orthorhombic $PbBiO_2Cl$ structure seen along its b_0 axis. The lead atoms are black; the bismuth are heavily outlined and book shaded. The still larger dot-and-line shaded circles are chlorine; atoms of oxygen are smaller and dotted.

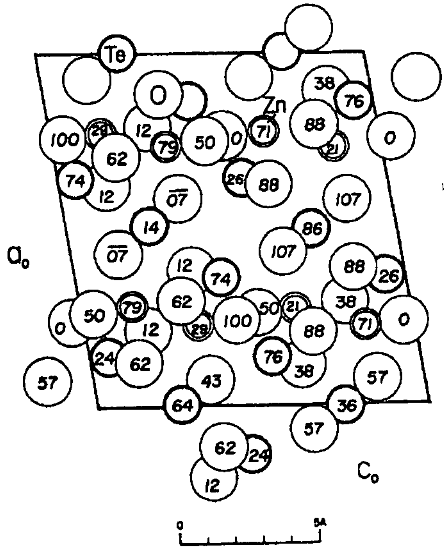
The resulting structure is shown in Figure XI,60. Each lead atom has four oxygen neighbors 2.45 A. away and four more distant chlorine atoms (3.25 and 3.30 A.). The environment of bismuth is similar, with Bi–4O = 2.27 A. and Bi–4Cl = 3.42 and 3.45 A.

The corresponding antimony compound, which occurs as the mineral *nadorite*, $PbSbO_2Cl$, is isostructural. For it:

$$a_0 = 5.59 \text{ A.}; \quad b_0 = 5.43 \text{ A.}; \quad c_0 = 12.20 \text{ A.}$$

The atomic positions and parameters are:

Pb: (4c) with $u = 0.380$
Sb: (4c) with $u = 0.078$
Cl: (4c) with $u = 0.756$
O: (8e) with $u = 0.25$



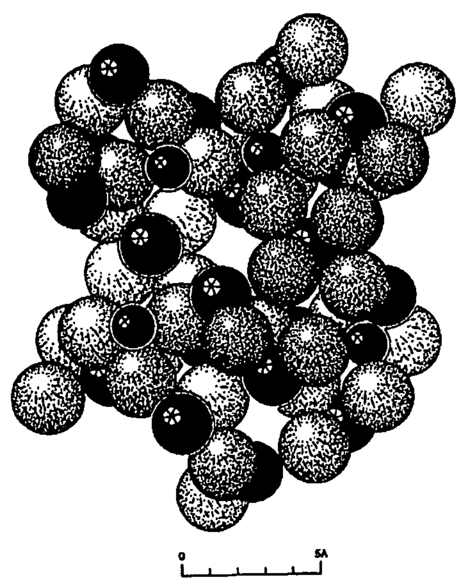


Fig. XI,90a (top). The monoclinic structure of $Zn_2Te_3O_8$ projected along its b_0 axis.
Fig. XI,90b (bottom). A packing drawing of the monoclinic structure of $Zn_2Te_3O_8$ seen along its b_0 axis. The zinc are the small, the tellurium the larger black circles. Atoms

BIBLIOGRAPHY TABLE, CHAPTER XI

Compound	Paragraph	Literature
$AgC(CN)_3$	2	1966: K&B
$AgCN\cdot 2AgNO_3$	1	1965: B&D
$Ag_{1-x}V_2O_5$	3	1965: A
$Ag_2O\cdot 4B_2O_3$	4	1965: KM
$AlBr_3\cdot H_2S$	6	1956: W,P&W
Al_4O_4C	7	1963: J&S
$Al_4Ta_3O_{13}(F,OH)$ (simpsonite)	9	1962: B&B
$Al_6B_5(OH)_3O_{15}$ (jeremejevite)	5	1934: G&K; 1938: S; 1955: G,B&B
$Al_5C_3N_3$	8	1963: J&W; 1966: J&W
$Al_7C_3N_3$	8	1963: J&W
$Al_8C_3N_4$	8	1963: J&W; 1966: J&W
$B_3S_3Br_3$	10	1958: Z
B_6H_9I	11	1965: H,B&P
BaB_4O_7	12	1965: B&P
$BaBi_2Nb_2O_9$	77	1949: A
$BaBi_4Ti_4O_{15}$	13	1950: A
$Ba_2TiNb_4O_{15}$	14	1965: S
$Ba_xBi_yO_z$	15	1943: A
Bi_3TaTiO_9	77	1949: A
Bi_3TiNbO_9	77	1949: A; 1960: I
$Bi_xRO_yX_z$	16	1938: S; 1939: S; 1940: S; 1941: S; S&GH; 1942: S; S&J; 1943: A; 1952: A
$CaB_3O_4(OH)$	17	1962: C,C&A
$CaBi_2Nb_2O_9$	77	1949: A; 1960: I
$CaBi_2Ta_2O_9$	77	1960: I
$Ca_{12}Be_{17}O_{29}$	18	1966: H&Y
$Ca_xBi_yO_z$	15	1943: A
CdB_4O_7	19	1966: I&KM
$CsB_{12}Be_4Al_4O_{28}$ (rhodizite)	20	1938: S; 1966: B&T
$Cs_3Re_3Br_{11}$	21	1965: E&P; 1966: E&P
$Cs_2UO_2Br_4$	22	1965: M,K&K
$Cs_2UO_2Cl_4$	23	1966: H,R&W
$Cs_2RhCl_5\cdot NH_4NO_3$	55	1944: Z&S
$Cs_x(UO_2)OCl_x$	24	1964: A&W
$CuCN\cdot N_2H_4$	26	1966: C,L&R
$CuPb_{13}Sb_7S_{24}$ (meneghinite)	27	1938: H; P,R&W; 1960: E&H

(continued)